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Extrapolation of G_0W_0 energy levels from small basis sets for elements from H to Cl TONG ZHU, VOLKER BLUM, MEMS Department, Duke University, Durham, NC 27708 — G_0W_0 calculations based on orbitals from a density-functional theory reference are widely used to predict carrier levels in molecular and inorganic materials. Their computational feasibility, however, is limited by the need to evaluate slow-converging sums over unoccupied states, requiring large basis sets paired with unfavorable scaling exponents to evaluate the self-energy. In the quantum chemistry literature, complete basis set (CBS) extrapolation strategies have been used successfully to overcome this problem for total energies. We here apply the principle of basis set extrapolation to G_0W_0 energy levels. For a set of 49 small molecules and clusters containing the elements H, Li through F, and Na through Cl, we test established extrapolation strategies based on Dunning's correlation-consistent (cc) basis sets (aug)-cc-pVNZ (N=2-5), as well as numeric atom-centered NAO-VCC-nZ (n=2-5) basis sets in the FHI-aims all-electron code. For the occupied and lowest unoccupied levels, different extrapolation strategies agree within ±50 meV based on large 4Z and 5Z basis sets. We show that extrapolation based on much smaller 2Z and 3Z basis sets with largest errors ± 100 meV based on a refinement of the NAO-VCC-nZ basis sets.

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